

ANEJO II

Primera Parte:

Esquema de los procesos metabólicos cinéticos con la formulación y las leyes que rigen cada uno:

Crecimiento**Heterótrofo (Ss) Aeróbico****Nutriente (NH₄⁺): 'Aer.GrowthHET(NH4)'**

$$[\text{Energía}] + S_s S_s + S_{\text{NH}_4} \text{NH}_4 + S_{\text{H}_2\text{O}} \text{H}_2\text{O} + S_{\text{HPO}_4} \text{HPO}_4 + S_{\text{O}_2} \text{O}_2 \rightarrow S_{\text{XH}} \text{XH} + S_{\text{HCO}_3} \text{HCO}_3 + S_{\text{H}} \text{H}$$

$$r_{\text{aer growth het (NH}_4)} = k_{\text{aer gro het}} \frac{S_s}{K_{S, \text{het}, \text{aer}} + S_s} \frac{O_2}{K_{O_2, \text{het}, \text{aer}} + O_2} \frac{NH_4}{K_{N, \text{het}, \text{aer}} + NH_4} \frac{HPO_4}{K_{HPO_4, \text{het}, \text{aer}} + HPO_4} \cdot X_H$$

Nutriente (NO₃⁻): 'Aer.GrowthHET(NO3)'

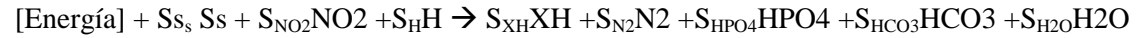
$$[\text{Energía}] + S_s S_s + S_{\text{NO}_3} \text{NO}_3 + S_{\text{HPO}_4} \text{HPO}_4 + S_{\text{O}_2} \text{O}_2 + S_{\text{H}_2\text{O}} \text{H}_2\text{O} \rightarrow S_{\text{XH}} \text{XH} + S_{\text{HCO}_3} \text{HCO}_3 + S_{\text{H}} \text{H}$$

$$r_{\text{aer growth het (NO}_3)} = k_{\text{aer gro het}} \frac{S_s}{K_{S, \text{het}, \text{aer}} + S_s} \frac{O_2}{K_{O_2, \text{het}, \text{aer}} + O_2} \frac{K_{N, \text{het}, \text{aer}}}{K_{N, \text{het}, \text{aer}} + NH_4} \frac{NO_3}{K_{N, \text{het}, \text{aer}} + NO_3} \left[\frac{HPO_4}{K_{HPO_4, \text{het}, \text{aer}} + HPO_4} \right] \cdot X_H$$

Heterótrofo (Ss) Anóxico**Oxidante (NO₃⁻): 'Anox.GrowthHET(NO3)'**

$$[\text{Energía}] + S_s S_s + S_{\text{NO}_3} \text{NO}_3 + S_{\text{H}_2\text{O}} \text{H}_2\text{O} + S_{\text{HPO}_4} \text{HPO}_4 \rightarrow S_{\text{XH}} \text{XH} + S_{\text{NO}_2} \text{NO}_2 + S_{\text{HCO}_3} \text{HCO}_3 + S_{\text{H}} \text{H}$$

$$r_{\text{anox growth het (NO}_3)} = k_{\text{anox gro het}} \frac{S_s}{K_{S, \text{het}, \text{anox}} + S_s} \frac{K_{O_2, \text{het}, \text{aer}}}{K_{O_2, \text{het}, \text{aer}} + O_2} \frac{NO_3}{K_{N, \text{het}, \text{anox}} + NO_3} \left[\frac{HPO_4}{K_{HPO_4, \text{het}, \text{anox}} + HPO_4} \right] \cdot X_H$$

Oxidante (NO₂⁻): 'Anox.GrowthHET(NO2)'

$$r_{\text{anoxgrowth}_{het}(NO_2)} = k_{\text{anoxgrohet}} \frac{S_s}{K_{S,het,anox} + S_s} \frac{K_{O_2,het,aer}}{K_{O_2,het,aer} + O_2} \frac{NO_2}{K_{NO_2,het,anox} + NO_2} \left[\frac{HPO_4}{K_{HPO_4,het,anox} + HPO_4} \right] \cdot X_H$$

Autótrofo (Fotosíntesis por algas)**Nutriente (NH₄⁺): 'GrowthALG(NH4)'**

$$r_{\text{growth}_{lg}(NH_4)} = k_{\text{groa}_{lg}} \frac{NO_3}{K_{NO_3,alg} + NO_3} \frac{NH_4}{K_{NH_4,alg} + NH_4} \frac{HPO_4}{K_{HPO_4,alg} + HPO_4} \cdot \left(\frac{I}{K_I} \exp \left(1 - \frac{I}{K_I} \right) \right) \cdot X_{alg}$$

I, es la radiación solar incidente (W/m²)

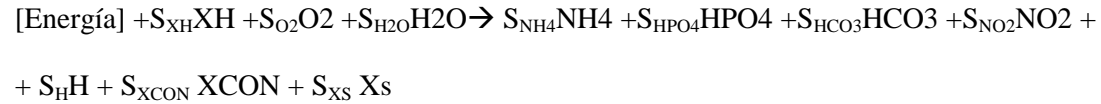
K_I, es la constante de radiación incidente

Nutriente (NO₃⁻): 'GrowthALG(NO3)'

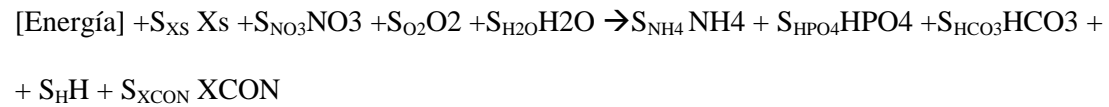
$$r_{\text{growth}_{lg}(NO_3)} = k_{\text{groa}_{lg}} \frac{NO_3}{K_{NO_3,alg} + NO_3} \frac{K_{NH_4,alg}}{K_{NH_4,alg} + NH_4} \frac{HPO_4}{K_{HPO_4,alg} + HPO_4} \cdot \left(\frac{I}{K_I} \exp \left(1 - \frac{I}{K_I} \right) \right) \cdot X_{alg}$$

I, es la radiación solar incidente (W/m²)

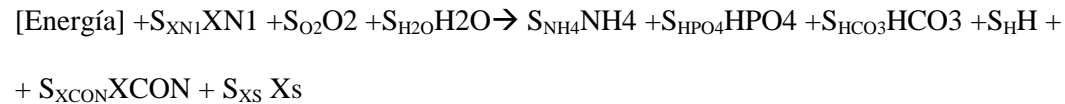
K_I, es la constante de radiación incidente

Consumo**de X_H :** 'GrowthCON(XH)'

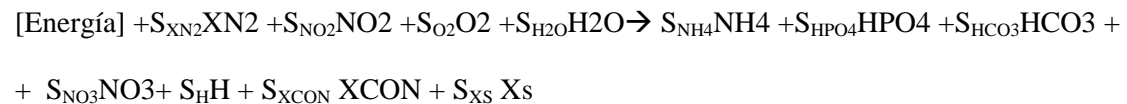
$$r_{gro,CON,Xh} = k_{gro,CON} \frac{O_2}{K_{O_2,CON} + O_2} \cdot X_{XH} \cdot X_{CON}$$

de X_S : 'GrowthCON(XS)'

$$r_{gro,CON,Xs} = k_{gro,CON} \frac{O_2}{K_{O_2,CON} + O_2} \cdot X_{XS} \cdot X_{CON}$$

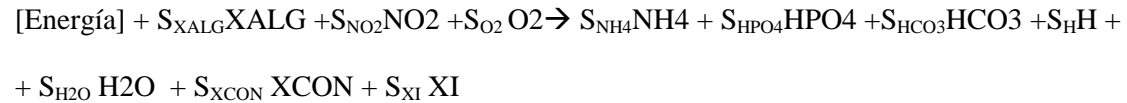
de X_{N1} : 'GrowthCON(XN1)'

$$r_{gro,CON,XN1} = k_{gro,CON} \frac{O_2}{K_{O_2,CON} + O_2} \cdot X_{XN1} \cdot X_{CON}$$

de X_{N2} : 'GrowthCON(XN2)'

$$r_{gro,CON,XN2} = k_{gro,CON} \frac{O2}{K_{O2,CON} + O2} \cdot X_{XN2} \cdot X_{CON}$$

de X_{ALG} : 'GrowthCON(ALG)'



$$r_{gro,CON,alg} = k_{gro,CON} \frac{O2}{K_{O2,CON} + O2} \cdot X_{alg} \cdot X_{CON}$$

Nitrificación

Reductor (NH_4^+): 'GrowthN1'



$$r_{anoxgrowN1} = k_{anoxgrowN1} \frac{O2}{K_{O2,N1,anox} + O2} \frac{NO3}{K_{NO3,N1,anox} + NO3} \cdot X_{N1}$$

Reductor (NO_2): 'GrowthN2'



$$r_{anoxgrowN2} = k_{anoxgrowN2} \frac{O2}{K_{O2,N2,anox} + O2} \frac{NO2}{K_{NO2,N2,anox} + NO2} \frac{HPO4}{K_{HPO4,N2,anox} + HPO4} \cdot X_{N2}$$

Respiración

Aerobia

X_H : 'Aer.Resp.HET'



$$r_{aerresphet} = k_{aerresphet} \frac{O2}{K_{O2,het,aer} + O2} \cdot X_H$$

X_{N1}: 'Aer.Resp.N1'



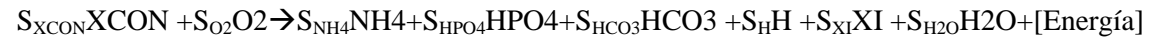
$$r_{anoxrespN1} = k_{anoxrespN1} \frac{O2}{K_{O2,N1} + O2} \cdot X_{N1}$$

X_{N2}: 'Aer.Resp.N2'



$$r_{anoxrespN2} = k_{anoxrespN2} \frac{O2}{K_{O2,N2} + O2} \cdot X_{N2}$$

X_{CON}: 'Aer.Resp.CON'

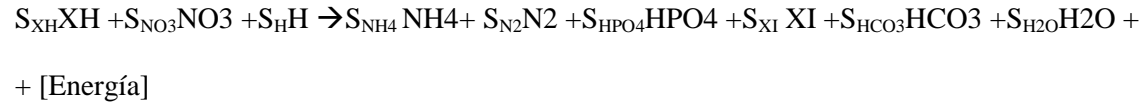


$$r_{resp,CON} = k_{resp,CON} \frac{O2}{K_{O2,CON} + O2} \cdot X_{CON}$$

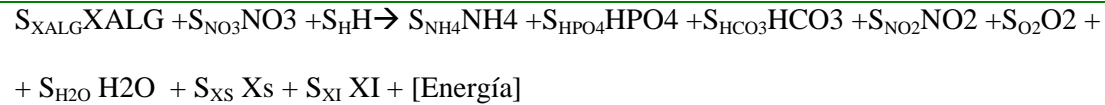
X_{ALG}: 'Aer.Resp.ALG'



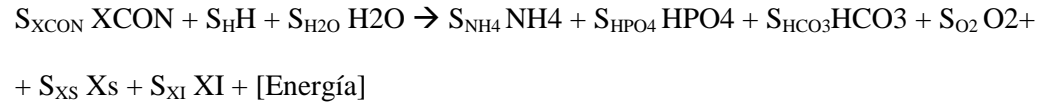
$$r_{resp,alg} = k_{resp,alg} \frac{O2}{K_{O2,alg} + O2} \cdot X_{alg}$$

Anóxica X_H : 'Anox.Resp.HET'

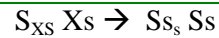
$$r_{anoxresphet} = k_{anoxresphet} \frac{S_s}{K_{S,het,anox} + S_s} \frac{NO_3}{K_{N,het,anox} + NO_3} \cdot X_H$$

Muerte X_{ALG} : 'DeathALG'

$$r_{death,alg} = k_{death,alg} \cdot X_{alg}$$

 X_{CON} : 'DeathCON'

$$r_{death,CON} = k_{death,CON} \cdot X_{CON}$$

Hidrólisis

$$r_{Hid} = k_{Hid} \cdot X_s$$

Segunda Parte:

Los coeficientes estequiométricos obtenidos y modelados en la tesina.

	'SS'	'NH4'	'NO2'	'NO3'	'HPO4'	'O2'	'HCO3'	'H'	'XH'	'XN1'	'XN2'	'XALG'	'XCON'	'XS'	'XI'	'H2O'	'N2'
	moles	moles	moles	moles	moles	moles	moles	moles	moles	moles	moles	moles	moles	moles	moles	moles	moles
Aer. Growth XH(NH4)	-1.67	-0.001			-0.0004	-0.043	0.0358	0.0364	1								-0.014
Aer. Growth XH(NO3)	-1.67			-0.001	-0.0004	-0.040	0.0358	0.0335	1								-0.020
Aer. Resp. XH		0.008			0.0009	-0.039	0.0332	0.0268	-1						0.20		-0.018
Anox. Growth XH(NO3)	-2.00		0.123	-0.123	-0.0003		0.0517	0.0510	1								-0.018
Anox. Growth XH(NO2)	-3.33		-0.187		0.0001		0.1150	-0.0720	1								-0.018
Anox. Resp. XH		0.008		-0.031	0.0009		0.0332	-0.0041	-1						0.20		-0.002
Growth XN1		-0.549	0.541		-0.0010	-0.761	-0.0433	1.0451		1							-0.002
Aer. Resp. XN1		0.008			0.0009	-0.039	0.0332	0.0268		-1					0.20		-0.014
Growth XN2			-2.381	2.372	-0.0010	-1.123	-0.0433	-0.0538			1						-0.020
Aer. Resp. XN2		0.008			0.0009	-0.039	0.0332	0.0268			-1				0.20		
Growth XALG(NH4)		-0.004			-0.0003	0.029	-0.0300	-0.0264				1					-0.006
Growth XALG(NO3)				-0.004	-0.0003	0.038	-0.0300	-0.0349				1					-0.008
Aer. Resp. XALG		0.004			0.0003	-0.017	0.0198	0.0165				-1			0.20		-0.014
Death XALG		0.002			0.0001	0.006	0.0001	-0.0015				-1		0.50	0.12		-0.011
Growth XCON(XALG)		0.009			0.0006	-0.004	0.0250	0.0177				-5	1	2.00		0.072	0.096
Growth XCON(XS)		0.009			0.0006	-0.139	0.1125	0.1052					1	-3.00		0.002	0.015
Growth XCON(XH)		0.030			0.0039	-0.111	0.0917	0.0694	-5				1	2.00		0.559	
Growth XCON(XN1)		0.030			0.0039	-0.111	0.0917	0.0694		-5			1	2.00		-0.014	
Growth XCON(XN2)		0.030			0.0039	-0.111	0.0917	0.0694			-5		1	2.00		0.009	
Aer. Resp. XCON		0.004			0.0003	-0.017	0.0198	0.0165					-1		0.20		-0.014
Death XCON		0.002			0.0001	0.006	0.0001	-0.0015					-1	0.50	0.12		0.002
Hydrolysis	1.00													-1.00			-0.002

